Effect of temperature history in the process on mechanical properties of thermoplastic resins and composites

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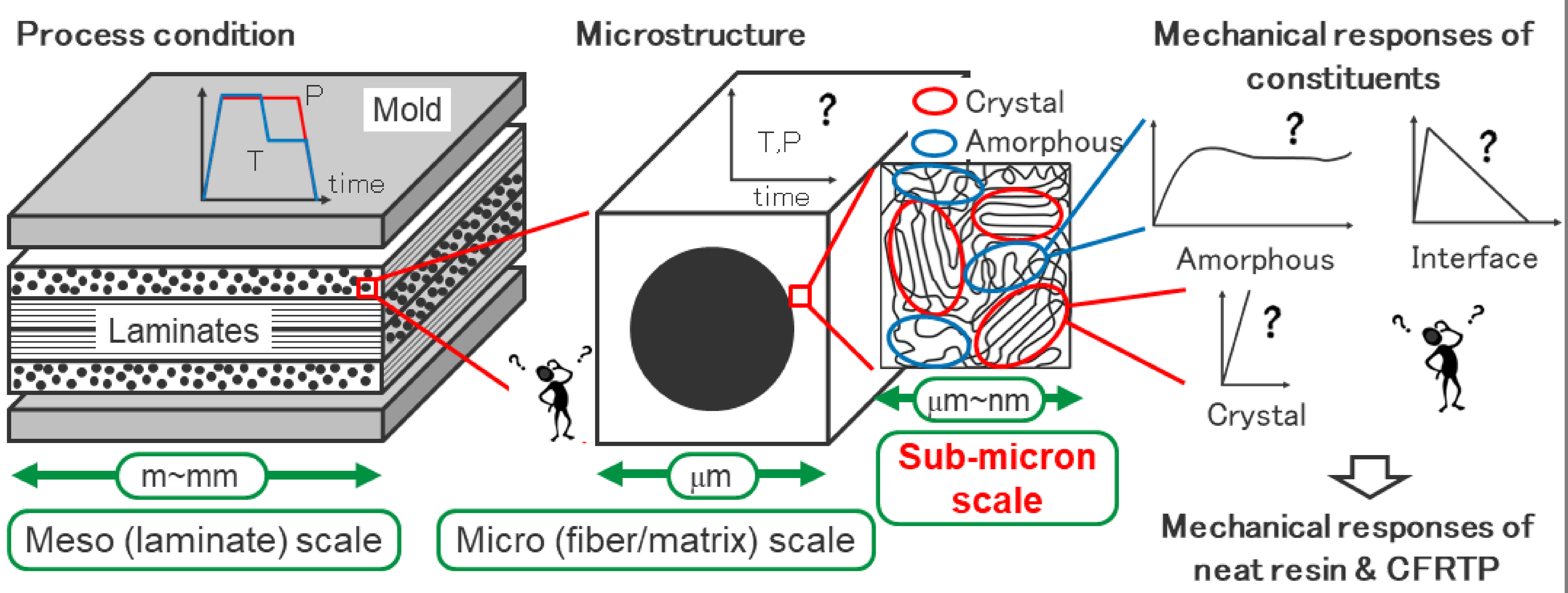
Introduction

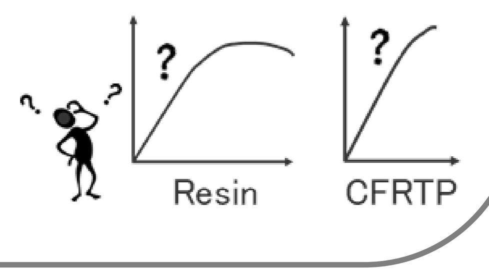
Carbon Fiber Reinforced ThermoPlastics (CFRTPs)

Advantage: Recyclability, Weldability, etc.

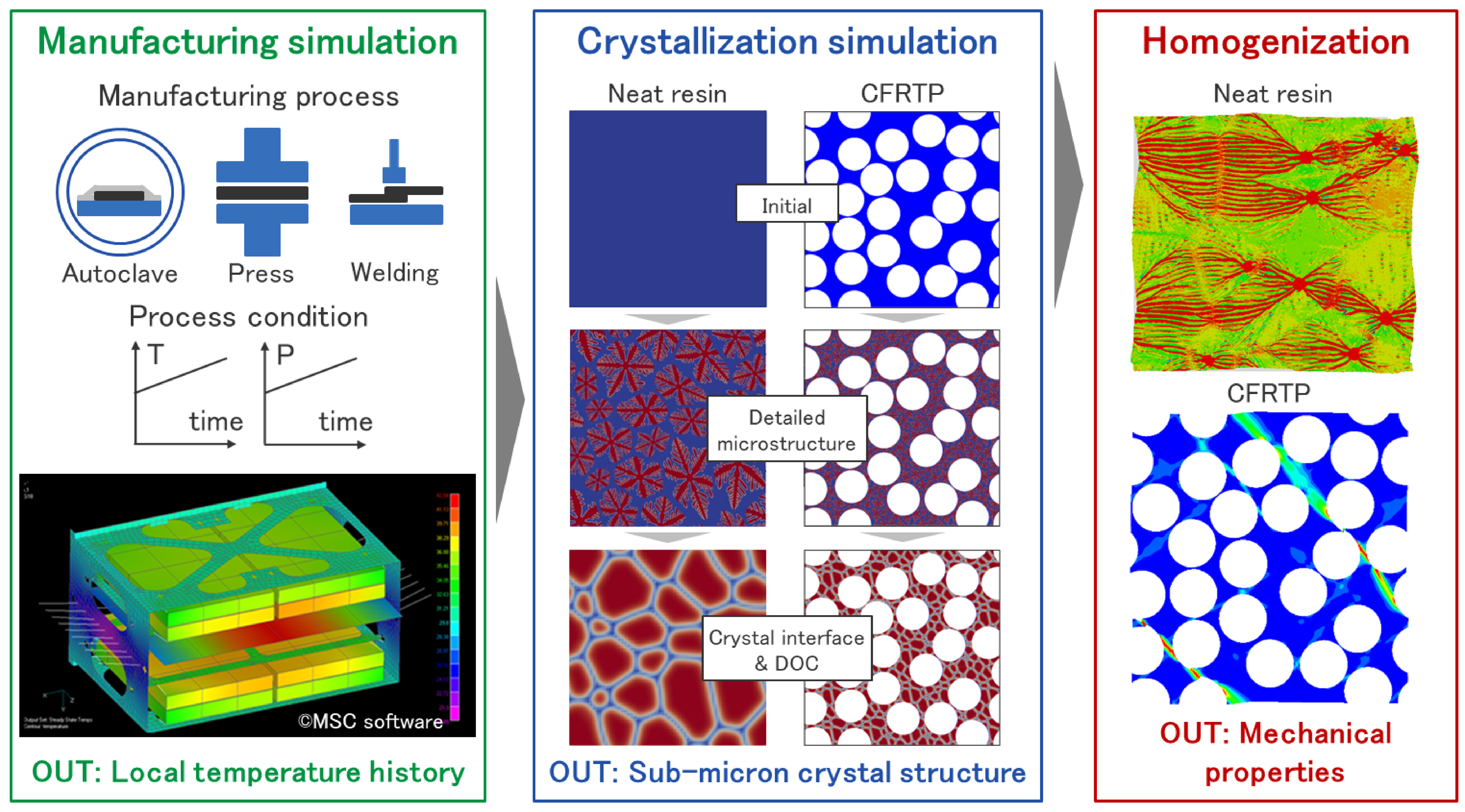
Disadvantage: Design and processing difficulty caused by **resin heterogeneity** (crystal & amorphous phases).



Numerical scheme to predict the process-dependent mechanical properties of thermoplastic resin and CFRTP is necessary.



Objective: To establish a multi-scale & multi-physics simulation scheme bridging from process conditions, through crystal structure, up to mechanical properties of thermoplastic resin and its composites.



Numerical method

Phase-field Crystallization simulation

- Phase-field variable ψ
  $\psi = 0$: Amorphous, $\psi = 1$: Crystal
- Total free energy of the system

$$F(\psi) = \int [f_{\mathrm{chem}}(\psi, T) + f_{\mathrm{surf}}(\psi)]\mathrm{d}V$$

Chemical free energy density

$$f_{\mathrm{chem}} = W\int_0^{\psi} \psi\left(\frac{1}{2} - \psi - m(T)\right)(1-\psi)\mathrm{d}\psi$$

with: $m(T) = \frac{a_k}{\pi}\arctan(\gamma(1-T))$

Surface free energy density

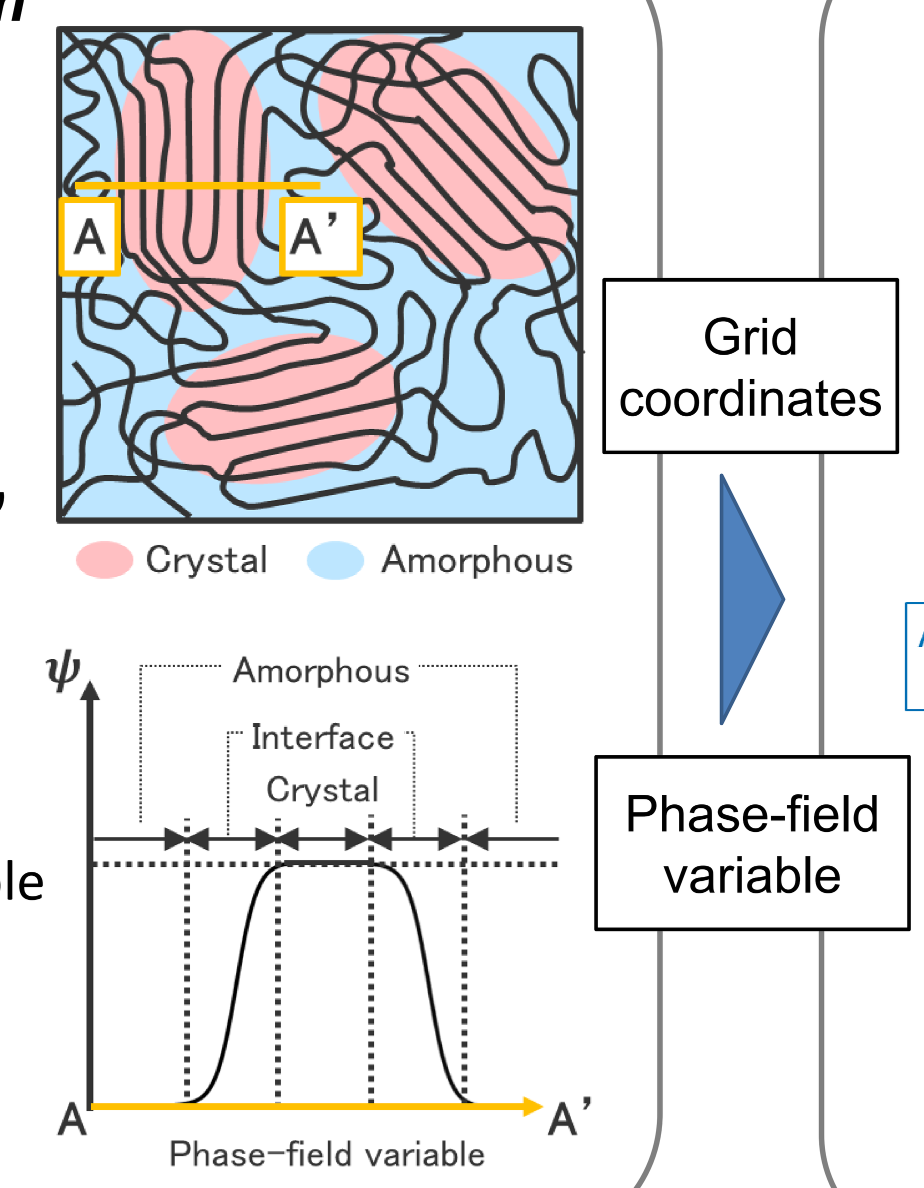
$$f_{\mathrm{surf}} = \frac{1}{2}\varepsilon^2(\nabla\psi)^2$$

- Temporal evolution of phase-field variable

$$\frac{\partial\psi(\boldsymbol{r},t)}{\partial t} = -M_{\psi}\frac{\delta F(\psi)}{\delta\psi(\boldsymbol{r},t)}$$

- Heat conduction

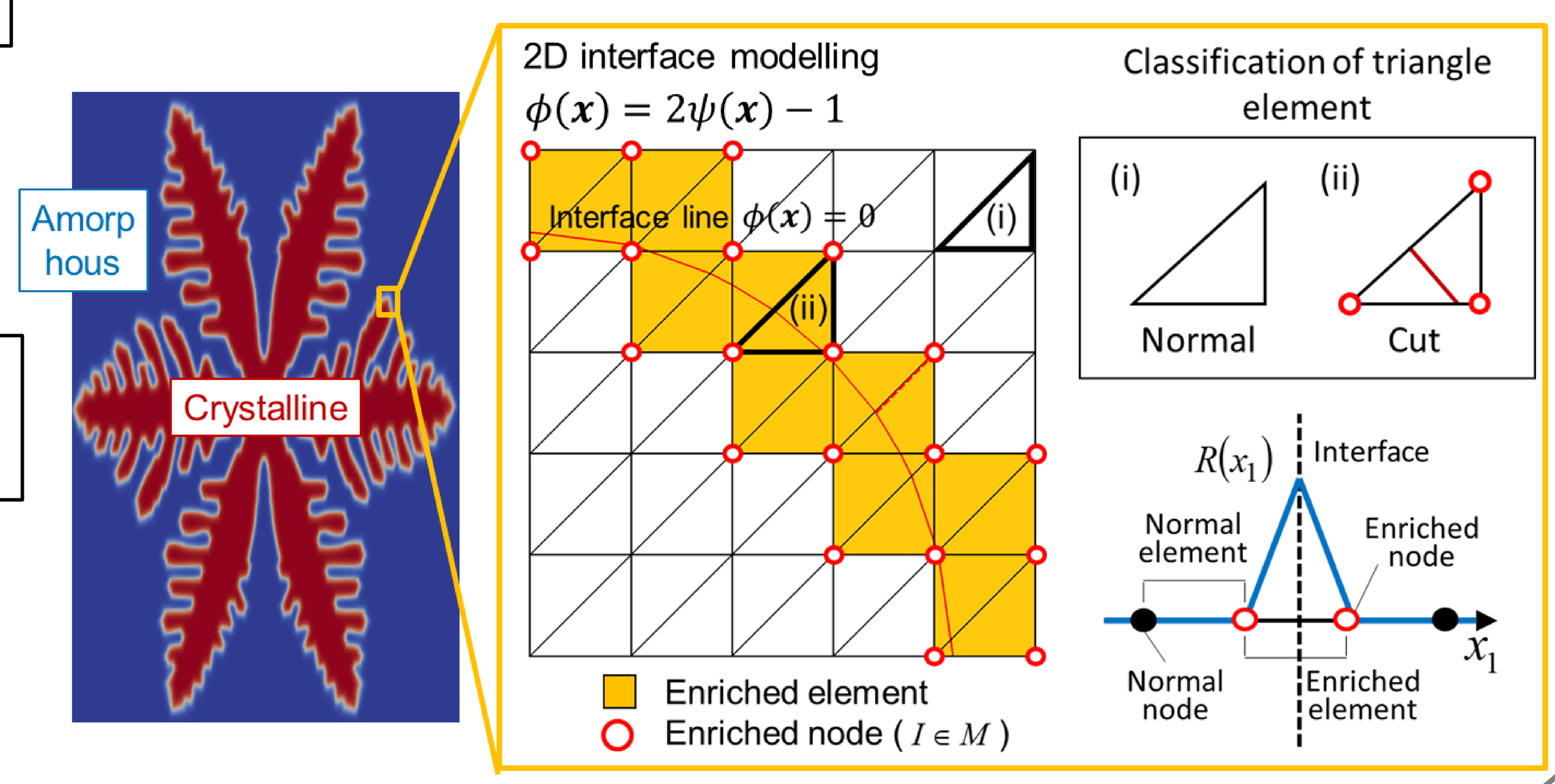
$$\rho C_{\mathrm{p}}\frac{\partial T}{\partial t} = k_{\mathrm{t}}\nabla^2 T + \rho\Delta H_{\mathrm{c}}\frac{\partial\psi}{\partial t}$$



Homogenization with eXtended Finite Element Method

XFEM can handle the discontinuity within one element by enrichment of shape function, and introduction of an additional degree of freedoms (DoFs).

Interpolation in XFEM: $\boldsymbol{u}^{\mathrm{h}}(\boldsymbol{x}) = \sum_{I=1}^{m} N_I(\boldsymbol{x})\boldsymbol{u}_I + \sum_{I\subseteq M} N_I(\boldsymbol{x})F(\boldsymbol{x})\boldsymbol{a}_I$

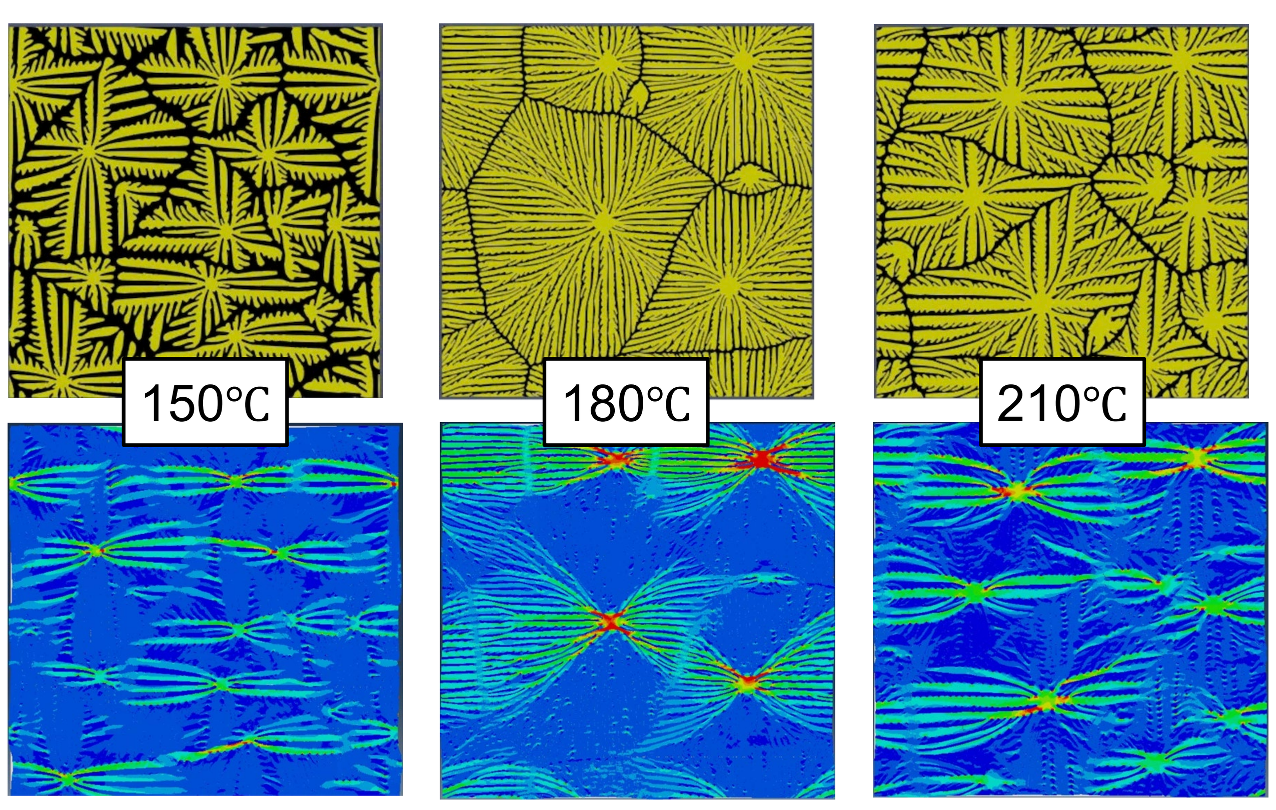


Results – Prediction of mechanical properties of thermoplastic resin

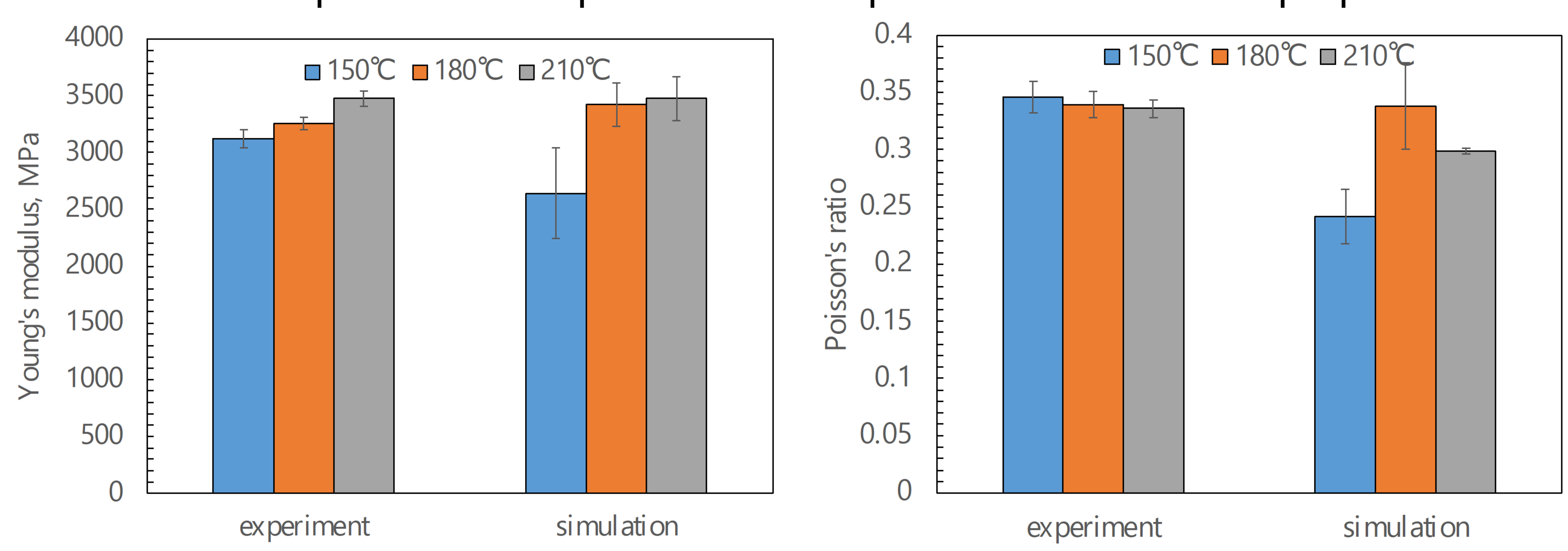
Conditions

- Material: Polyphenylene Sulfide (PPS)
- Temperature: 150℃, 180℃, 210℃ (isothermal)
- Loading: Unit strain in x-direction

Results (Top: Crystal morphologies obtained by phase-field method, Bottom, Stress distribution predicted by homogenization)



Results: Comparisons of experimental and predicted mechanical properties



- The predicted lamella thickness increased with the crystallization temperature, which is the same trend as that of the degree of crystallinity in the experiment.
- The proposed scheme was able to predict the mechanical properties of neat PPS resin qualitatively.

The proposed scheme is useful to grasp the trend of process-dependent mechanical properties of thermoplastic resin and CFRTP in the design process.